Momentum Average Approximations for single polarons

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Polarons:

Consider a typical lattice model description of electron-phonon interactions:

$$H = \sum_k \varepsilon_k c_k^+ c_k + \Omega \sum_q b_q^+ b_q + \frac{1}{\sqrt{N}} \sum_{k,q} g(q) c_{k-q}^+ c_q (b_q^+ + b_{-q})$$

I will only discuss **single polaron physics at T=0**.

Results shown here are for a simple cubic-like lattice + nn hoping, and
→ Holstein model in d=1, 2, 3, with g(q) = g
→ 1D breathing phonon mode model, where g(q) ~ sin(qa/2)

This approach can be generalized with the same level of accuracy to models with complex lattices (several electronic bands), multiple Einstein phonon modes, also to some g(k,q) couplings

Three energy scales → two dimensionless parameters: effective coupling + adiabaticity parameter

$$\lambda = \frac{\left\langle |g(q)|^2 \right\rangle}{2dt\Omega}, \quad \frac{\Omega}{2dt}$$

Quantity of interest: the Green's function G(k,ω) and the spectral weight A(k,ω)

$$H\left|1,k,\alpha\right\rangle = E_{1,k,\alpha}\left|1,k,\alpha\right\rangle$$

← eigenenergies and eigenfunctions (1 electron, total momentum k, α is collection of other quantum numbers)

$$G(k,\omega) \triangleq \left\langle 0\right| c_k \frac{1}{\omega - H + i\eta} c_k^+ \left|0\right\rangle = \sum_\alpha \frac{Z_{1,k,\alpha}}{\omega - E_{1,k,\alpha} + i\eta}$$

$$Z_{1,k,\alpha} = \left|\left\langle 1,k,\alpha\right| c_k^+ \left|0\right\rangle\right|^2$$

$$A(k,\omega) \triangleq -\frac{1}{\pi} \operatorname{Im} G(k,\omega)$$

← measured in (inverse) ARPES, also linked to LDOS measured by STM

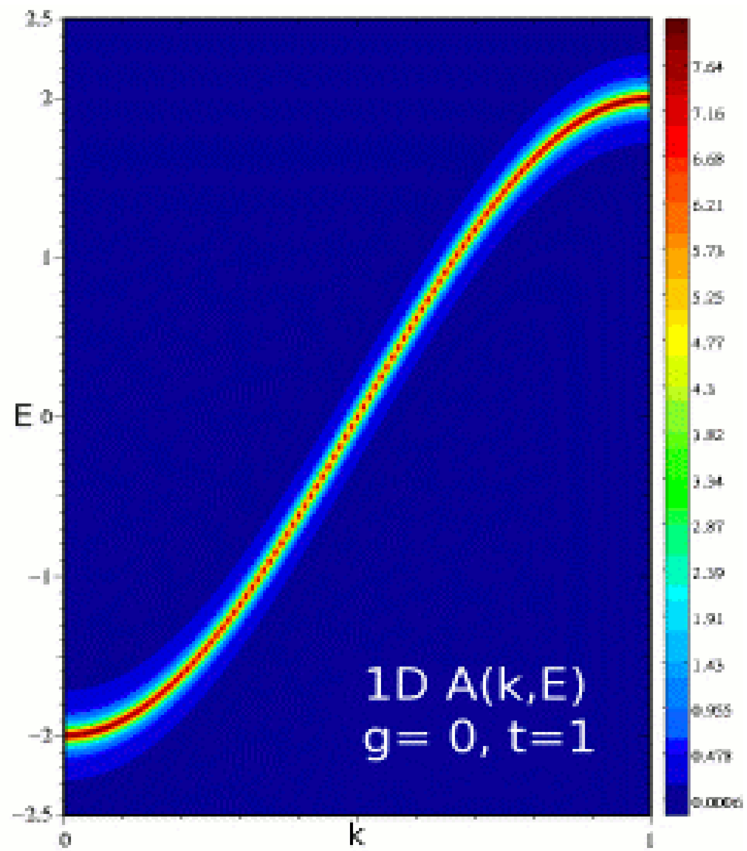
Holstein model:

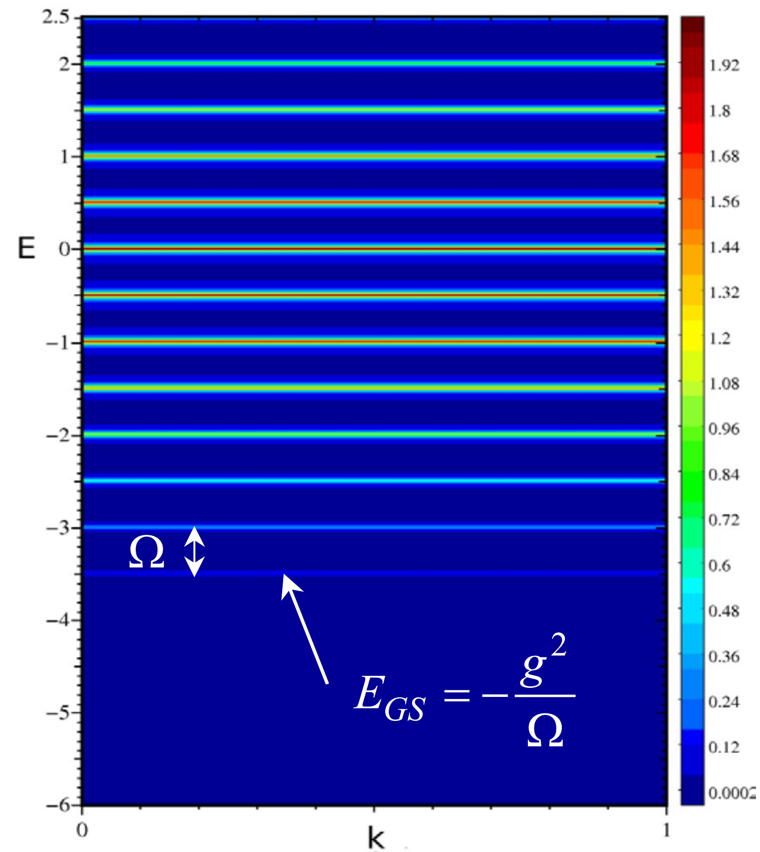
weak coupling $\lambda = \frac{g^2}{2dt\Omega} = 0 \quad (g = 0)$

$$G_0(k,\omega) = \frac{1}{\omega - \varepsilon_k + i\eta};$$

Lang-Firsov impurity limit $\lambda = \frac{g^2}{2dt\Omega} = \infty \quad (t = 0)$

$$G_{LF}(k,\omega) = e^{-\frac{g^2}{\Omega^2}} \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{g}{\Omega}\right)^{2n} \frac{1}{\omega + \frac{g^2}{\Omega} - n\Omega + i\eta}$$

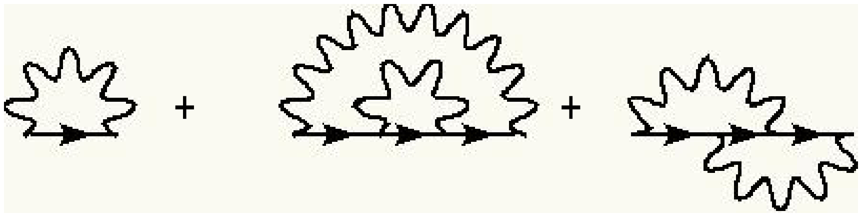




How does the spectral weight evolve between these two very different limits?

Calculating the Green's function:

$$G(k,\omega) = \frac{1}{\omega - \varepsilon_k - \Sigma(k,\omega) + i\eta} \qquad G_0(k,\omega) = \frac{1}{\omega - \varepsilon_k + i\eta}$$

Σ(k,ω) =  +….

For these polarons, we need to sum to orders well above $\langle g^2\rangle/\Omega^2$ to get convergence.

n	1	2	3	4	5	6	7	8
Σ, exact	1	2	10	74	706	8162	110410	1708394
Σ, SCBA	1	1	2	5	14	42	132	429

Traditional approach: find a subclass of diagrams that can be summed, ignore the rest

→ self-consistent Born approximation (SCBA) – sums only non-crossed diagrams (much fewer)

New approach: the MA$^{(n)}$ (momentum average) hierarchy of approximations:

Idea: → generate the infinite hierarchy of coupled equations of motion for the propagator (BBGKY)

→ keep all of them instead of truncating and factorizing

→ simplify by ignoring terms that are exponentially small

→ can solve the resulting equations analytically to find the self-energy

Depending on the level where we start making approximations → n in MA$^{(n)}$

Equivalent to analytical summation of ALL self-energy diagrams after discarding exponentially small contributions to each of them.

Results are EXACT in both asymptotic limits (zero el-ph coupling and zero bandwidth) and computationally trivial to evaluate for any values of the parameters.

Eg: MA$^{(0)}$ self-energy for the Holstein model: $$\Sigma_{MA^{(0)}}(\omega) = \cfrac{g^2 g_0(\omega-\Omega)}{1-\cfrac{2g^2 g_0(\omega-\Omega)g_0(\omega-2\Omega)}{1-\cfrac{3g^2 g_0(\omega-2\Omega)g_0(\omega-3\Omega)}{\cdots}}}$$

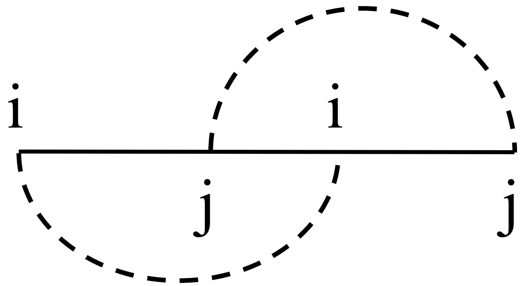
$$g_0(\omega) = \frac{1}{N}\sum_{\vec{k}} G_0(\vec{k},\omega) = \int_{B.Z.} \frac{d\vec{k}}{(2\pi)^d}\frac{1}{\omega-\varepsilon_{\vec{k}}+i\eta}$$

Note: for a model with g(q) dependence, the **MA self-energy is momentum dependent** for all n.

for Holstein model, momentum dependence appears only for n=2 and higher.

What does this mean?

(i) Real-space argument: MA$^{(0)}$ means $G_0(i-j,\omega) \to \delta_{i,j} G_0(0,\omega) = \delta_{i,j} g_0(\omega)$



$$exact: \quad \frac{g^4}{N^2} \sum_{i,j} G_0(j-i,\omega-\Omega) G_0(i-j,\omega-2\Omega) G_0(j-i,\omega-\Omega)$$

$$MA^{(0)}: \; g^4 g_0(\omega-\Omega) g_0(\omega-2\Omega) g_0(\omega-\Omega)$$

At low energies $\omega \sim E_{GS} < -2dt$ → free electron Greens' functions decrease exponentially with distance |i-j| → MA$^{(0)}$ keeps the most important (diagonal) contribution. The approximation becomes better the more phonons are present, since the lower $\omega - n\,\Omega$ is, the faster the decay.

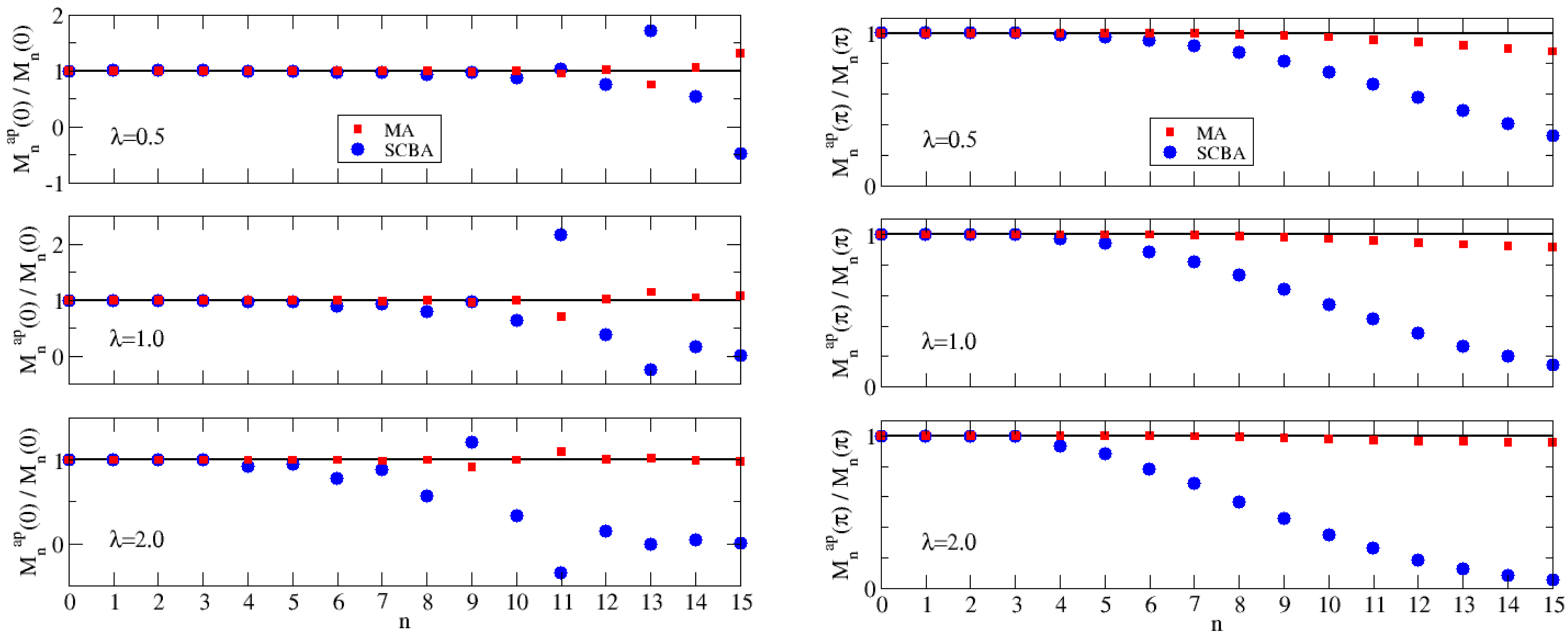
(ii) Spectral weight sum rules (see PRB 74, 245104 (2006) for details)

$$M_n(k) = \langle 0 | c_k H^n c_k^+ | 0 \rangle = \int_{-\infty}^{\infty} d\omega \omega^n A(k,\omega) = -\frac{1}{\pi} \mathrm{Im} \int_{-\infty}^{\infty} d\omega \omega^n G(k,\omega)$$

Keeping correct no. of diagrams is extremely important → MA$^{(0)}$ satisfies exactly sum rules up to n=5, and is highly accurate for all higher n (predicts correctly the most important terms);

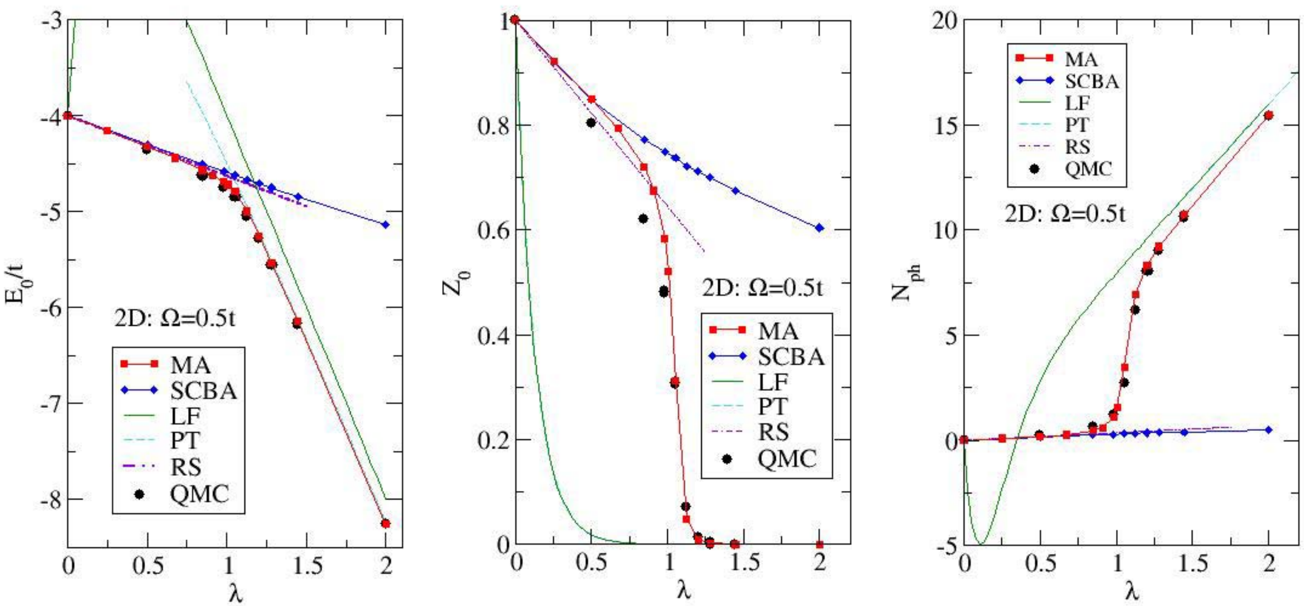
MA$^{(1)}$ is exact up to n=7, MA$^{(2)}$ is exact up to n=9, …

Ratios of sum rules for MA$^{(0)}$ (red) and SCBA (blue) wrt exact sum rules, Holstein, 1D



$$\lambda = \frac{g^2}{2dt\Omega}$$

Lots of comparison against numerical results, agreement very good unless the phonon frequency is very small. Moreover, it can be systematically improved. [PRL 97, 036402 (2006); PRB 74, 245104 (2006); PRL 98, 209702 (2007); PRB 76, 165109 (2007), Can. J. Phys 86, 523 (2008)].



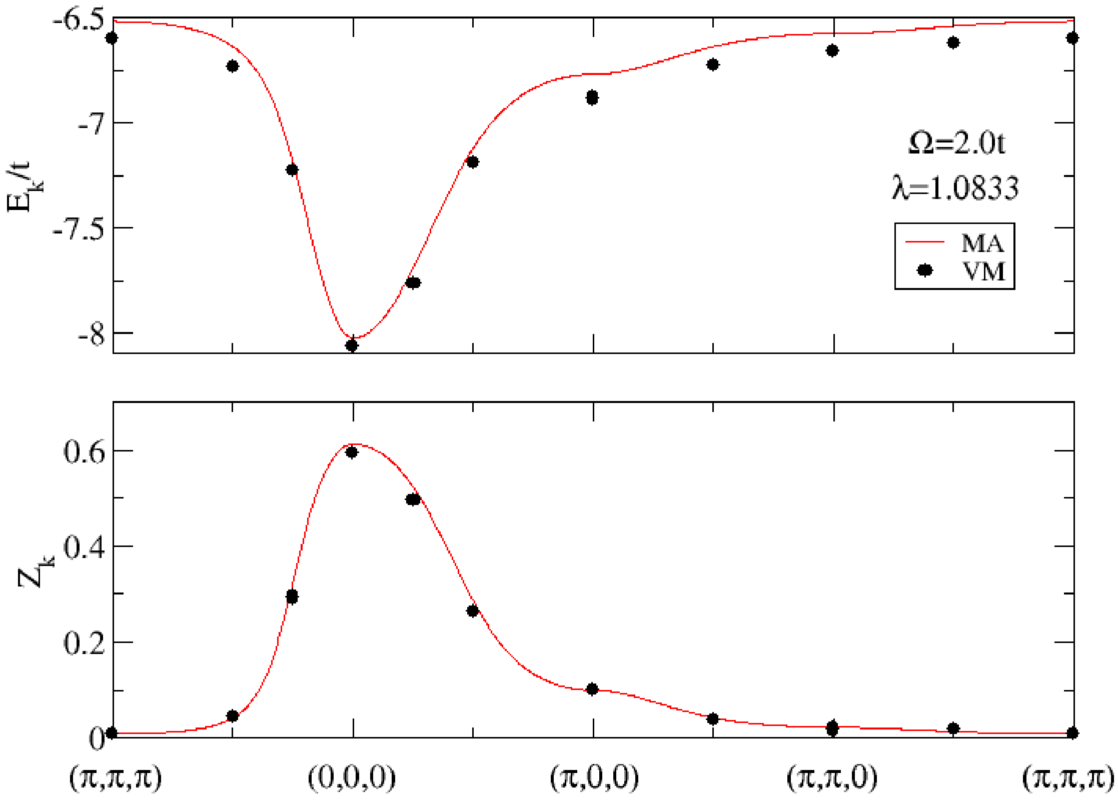
Results for the polaron ground state (a) energy; (b) quasiparticle weight; (c) average number of phonons in the polaron cloud, vs. λ

Black circles are Quantum Monte Carlo data, red squares are MA predictions, other curves are various other known approximations

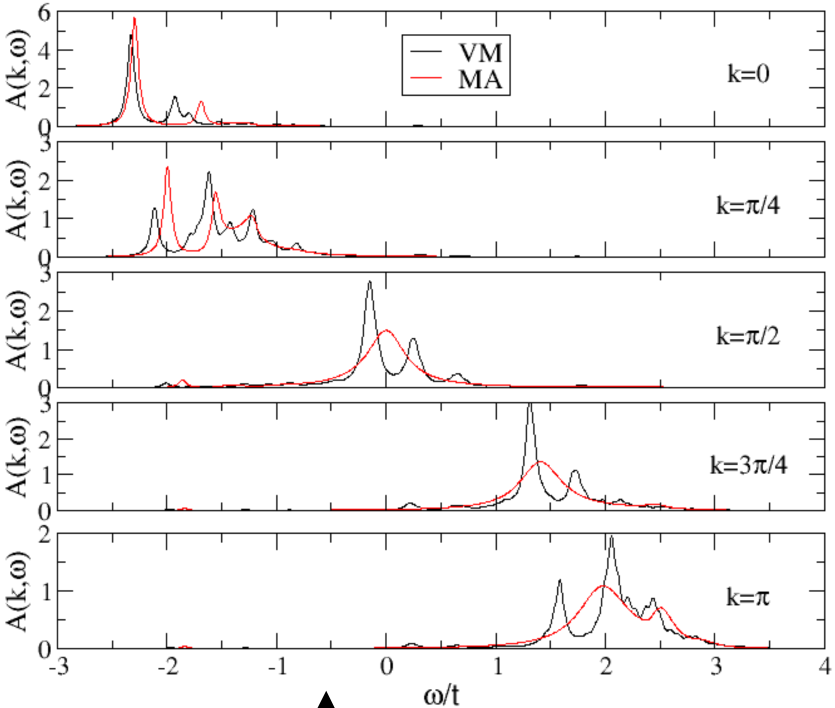
$$\lambda = \frac{g^2}{2dt\Omega}$$

is the effective coupling strength

3D Polaron dispersion

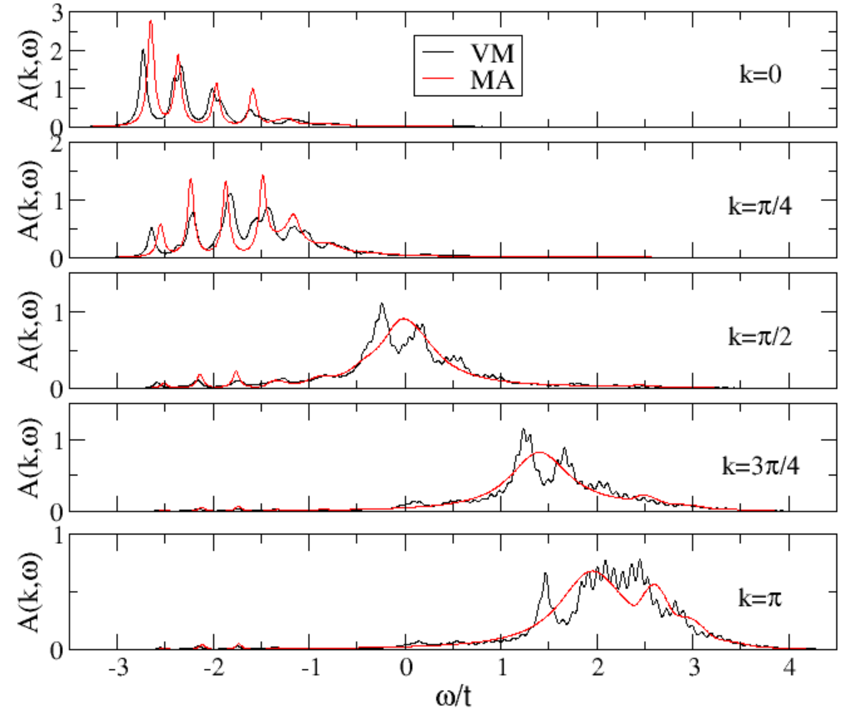


L. -C. Ku, S. A. Trugman and S. Bonca, Phys. Rev. B 65, 174306 (2002).

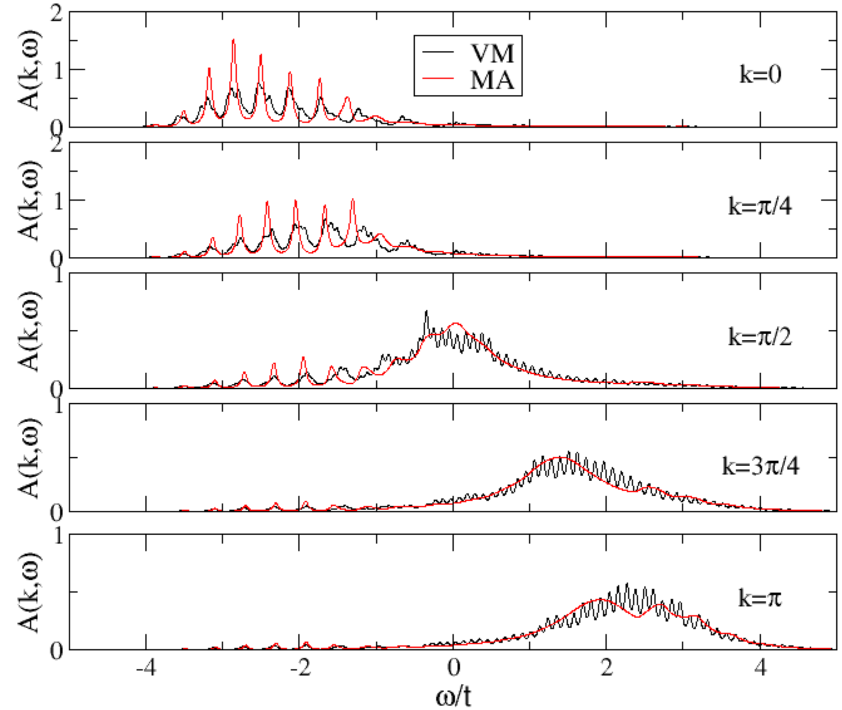


λ = 0.5

λ = 1



λ = 2

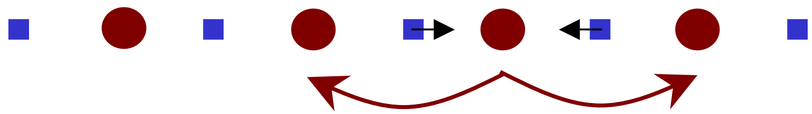


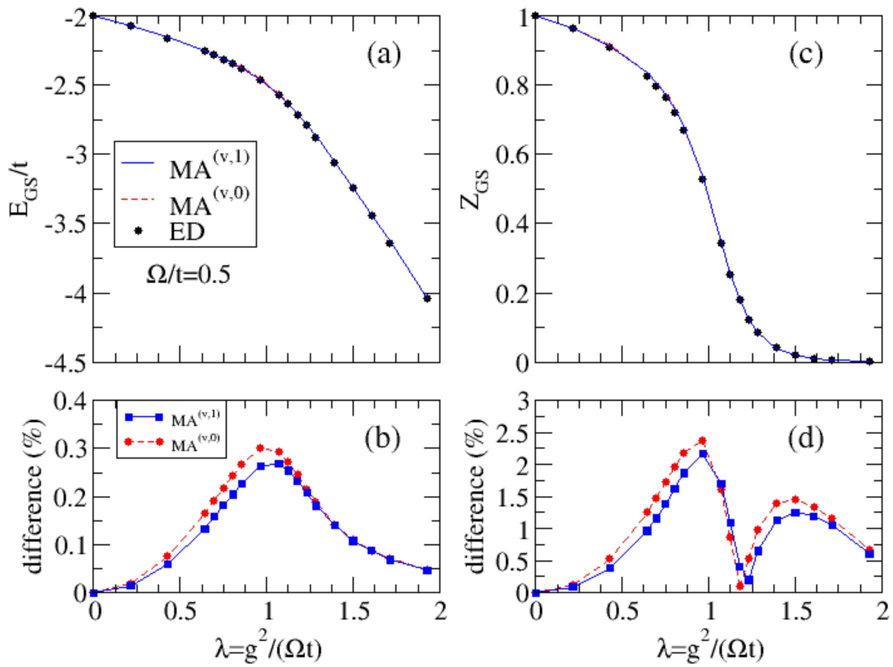
A(k,ω) in 1D

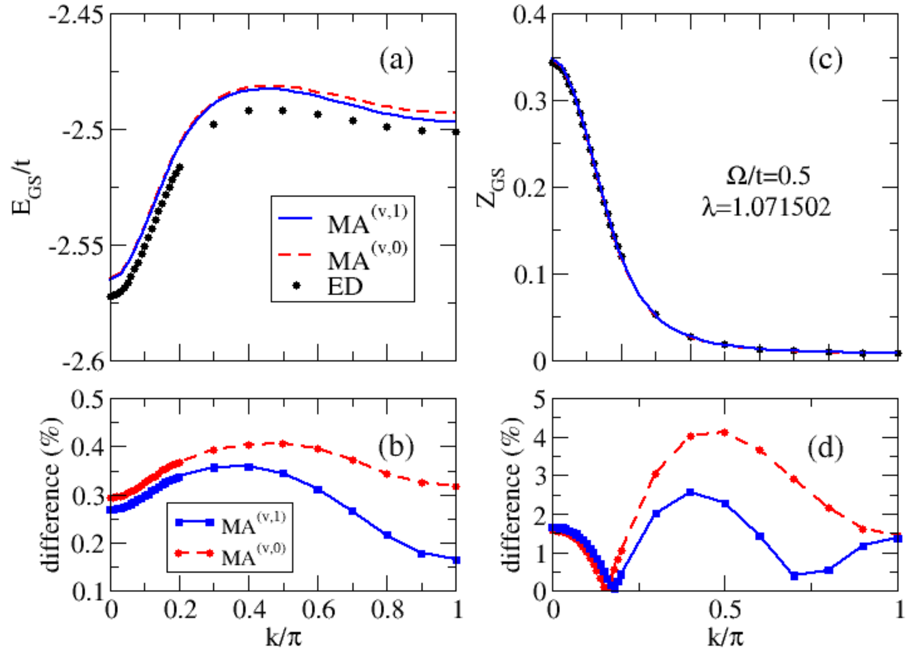
G. De Filippis et al, PRB 72, 014307 (2005)

MA becomes exact for small, large λ

Coupling to breathing-mode phonon: $g(q) \propto i \sin\frac{qa}{2}$







$$E_P(k) \sim t_{1,eff} \cos(ka) + t_{2,eff} \cos(2ka) + \ldots$$

Numerics: Bayo Lau, M. Berciu and G. A. Sawatzky, Phys. Rev. B 76, 174305 (2007)

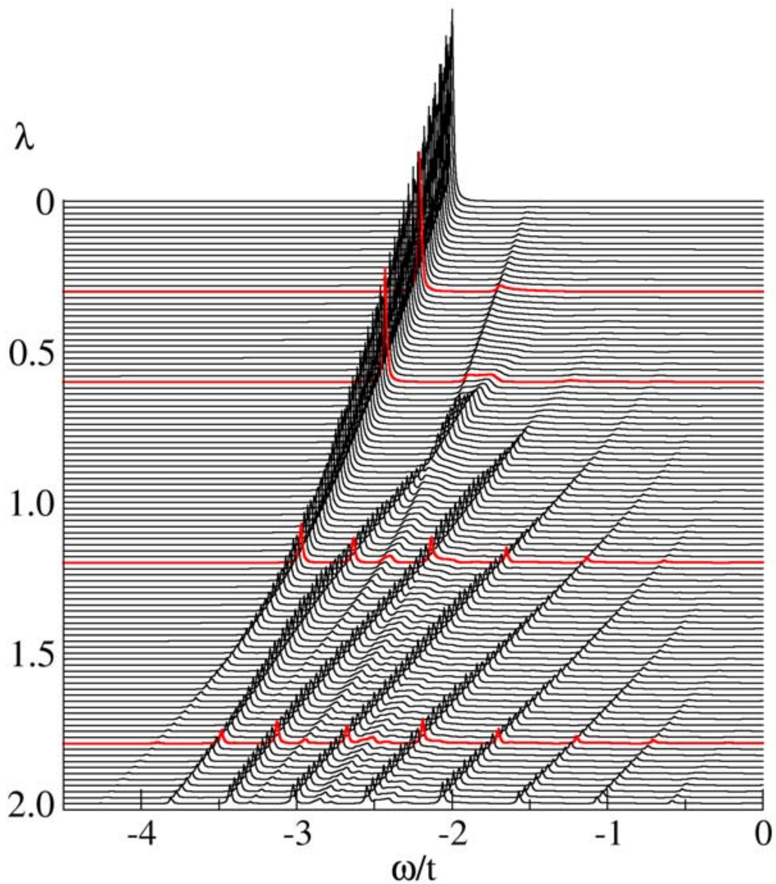
MA: Glen L. Goodvin and M. Berciu, Phys. Rev. B 78, 235120 (2008)

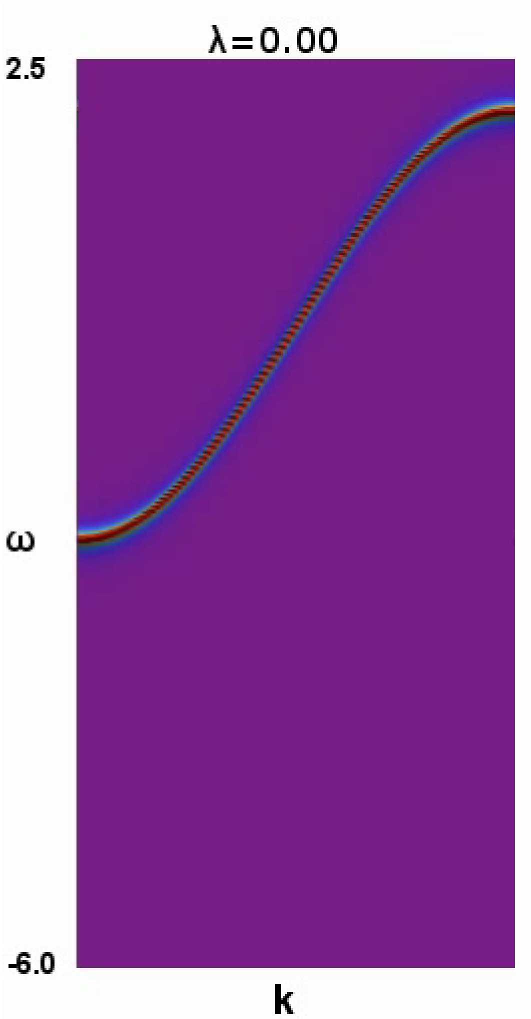
Many more things to say, eg about the (quasi)-variational meaning of these approximations, need to go to $MA^{(1)}$ or higher to properly capture polaron+phonon continuum, etc.

Conclusion so far:

→ It is an approximation (not exact), however it is accurate enough and easy to use to allow one to explore quickly all parameter space and the whole energy spectrum to understand the polaron's properties.

MA(2) results for Holstein.





1D, k=0, Ω=0.5t

Note: color scale is not linear!

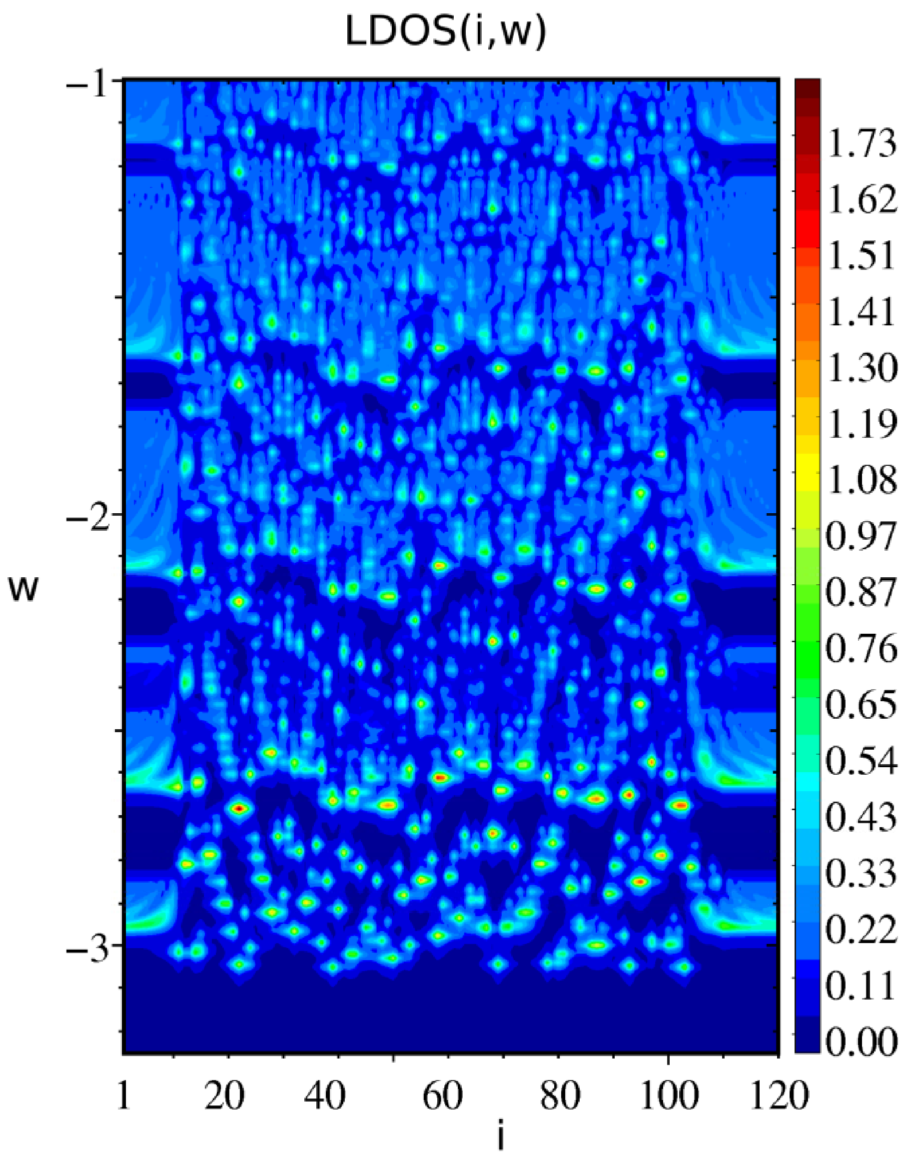
Since the initial work for Holstein model, we have been successful in generalizing to

→ Holstein models with multiple phonon bands and/or complex latttices [L. Covaci and M. Berciu, EPL 80, 67001, (2007); graphene → PRL 100, 256405 (2008); spin-orbit coupling → PRL 102, 185403 (2009)]

→ generalizations to models with electron-phonon coupling g(q) [G.L. Goodvin and M. Berciu, PRB 78, 235120 (2008)]

→ systems with broken translational invariance:

→ by disorder – either electronic on-site potentials, and/or inhomogeneities in the el-ph coupling or in the phonon frequencies (M. Berciu, A. Mishchenko, N. Nagaosa, arXiv:0609:1233)



t = 1; Ω =0.5; g=1.1 → λ =1.21

Sites 10-110: 1.05 < g < 1.15

Can also add inhomog. for Ω, t, on-site potentials, etc

Note: instantaneous approximations work very poorly if el-ph coupling is strong, because the el-ph interaction also renormalizes strongly (+ retardation) the impurity potential.

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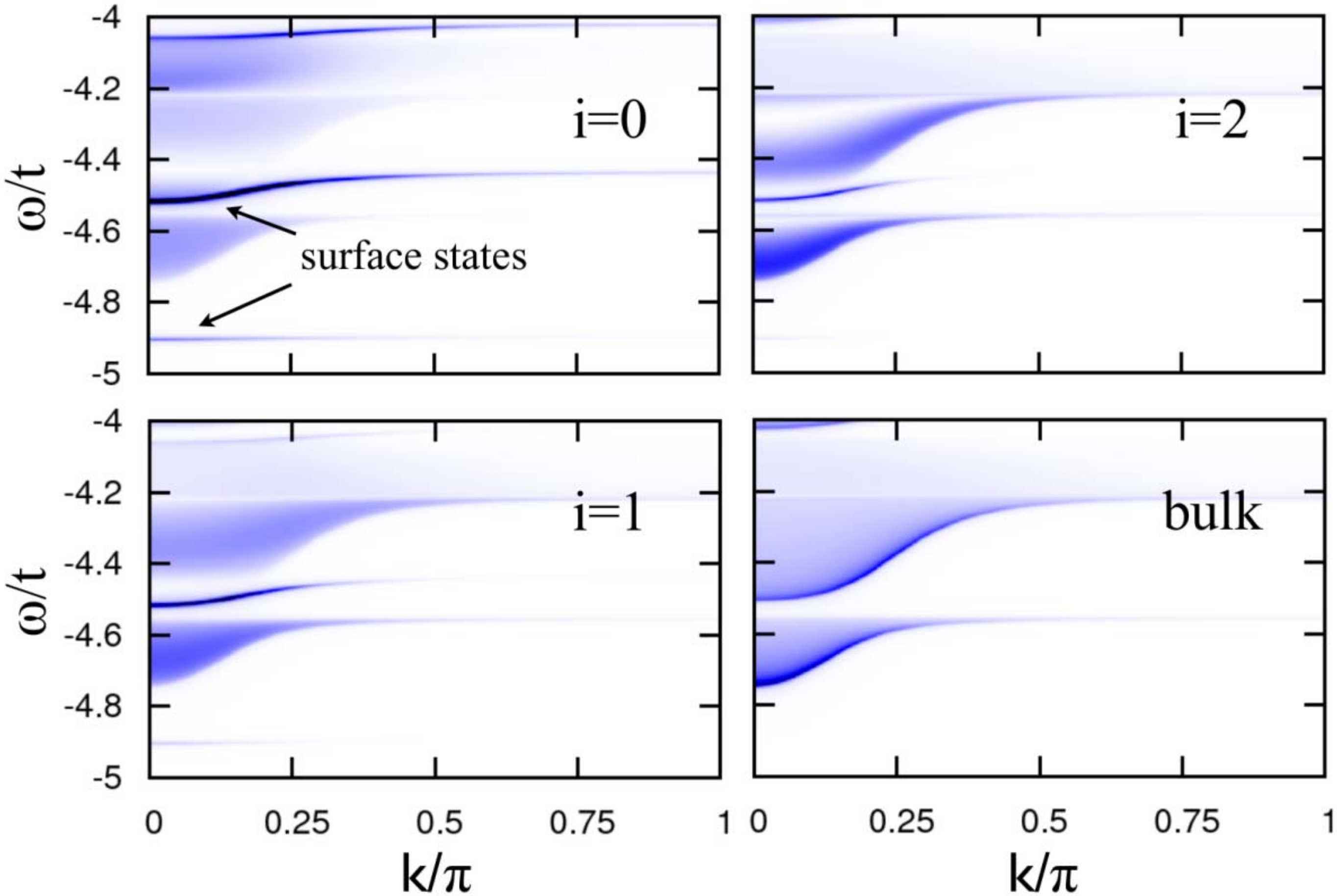

i=0
i=2
i=1
bulk
surface states
ω/t
k/π
-4
-4.2
-4.4
-4.6
-4.8
-5
0
0.25
0.5
0.75
1

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→ under way: optical absorption, g(k,q) models (phonon-modulated hopping); finite-T, bipolarons …

→ stumble upon exactly solvable models [M. Berciu, PRB 75, 081101(R) (2007); M. Berciu and G. A. Sawatzky, EPL 81, 57008 (2008)]

→ with George Sawatzky, work on spin-polarons (M. Berciu and G. A. Sawatzky, PRB 79, 195116 (2009)), electronic-polarons (next talk, PRB 79, 214507 (2009)), ….